Supporting information for: Conformational Preferences of *trans*-1,2- and *cis*-1,3-Cyclohexanedicarboxylic Acids in Water and DMSO as a Function of Ionization State as Determined from NMR Spectroscopy and DFT Quantum Mechanical Calculations

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Experimental and Computed Spectra

All spectra were measured at 600 MHz with temperature regulated at 25°C. Typical running conditions of the spectrometer were as follows: 1H spectra, 16 scans, spectral width 9600 Hz, relaxation delay 1 second and 4 seconds of acquisition time.

Spectra of trans-1,2-CDCA in D_2O

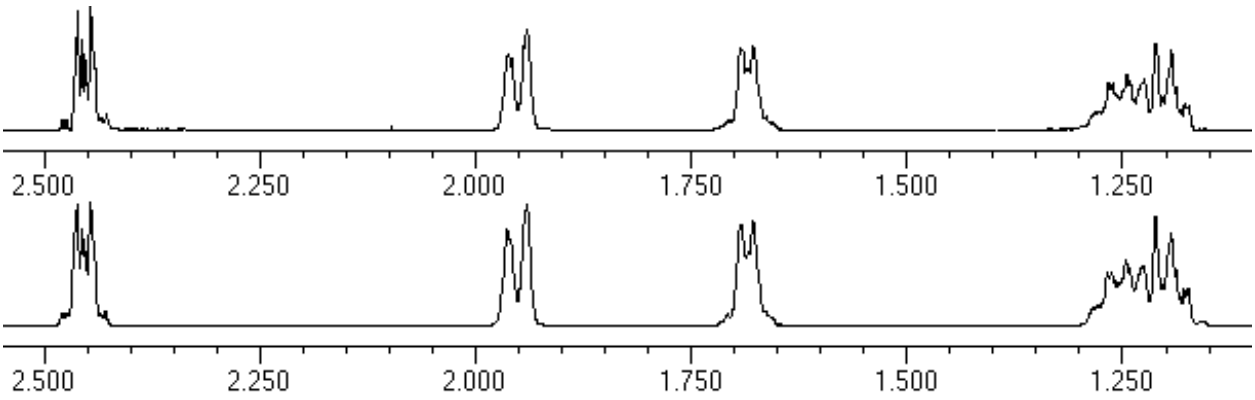

Figure 1: The experimental and simulated ^{1}H NMR spectra of *trans*-1,2-CDCA in D_2O at pH = 1.88. The bottom spectrum is the computed one.

#	Nucleus	n	Shift	Width	J[1]	J[2]	J[3]	J[4]	J[5]	J[6]	J[7]	J[8]	J[9]
1	1H	1	2.454										
			A	-									
2	1H	1	1.951		3.93								
			B	-	AB								
3	1H	1	1.253		12.49	-13.30							
			C	-	AC	BC							
4	1H	1	1.684		-0.90	2.88	3.62						
			D	-	AD	BD	CD						
5	1H	1	1.196		0.07	3.66	13.01	-13.66					
			E	-	AE	BE	CE	DE					
6	1H	1	2.454		10.83	-0.50	0.14	0.00	0.00				
			F	-	AF	AG	AH	AI	AJ				
7	1H	1	1.951		-0.50	0.00	0.00	1.22	-0.59	3.93			
			G	-	AG	BG	BH	BI	BJ	AB			
8	1H	1	1.253		0.14	0.00	0.00	0.00	0.03	12.49	-13.30		
			H	-	AH	BH	CH	CI	CJ	AC	BC		
9	1H	1	1.684		0.00	1.22	0.00	2.62	3.58	-0.90	2.88	3.62	
			I	-	AI	BI	CI	DI	DJ	AD	BD	CD	
10	1H	1	1.196		0.00	-0.59	0.03	3.58	12.96	0.07	3.66	13.01	-13.66
			J	-	AJ	BJ	CJ	DJ	EJ	AE	BE	CE	DE

Figure 2: The chemicals shifts and coupling constants for the computed ^{1}H NMR spectrum of *trans*-1,2-CDCA in D_2O at pH = 1.88.

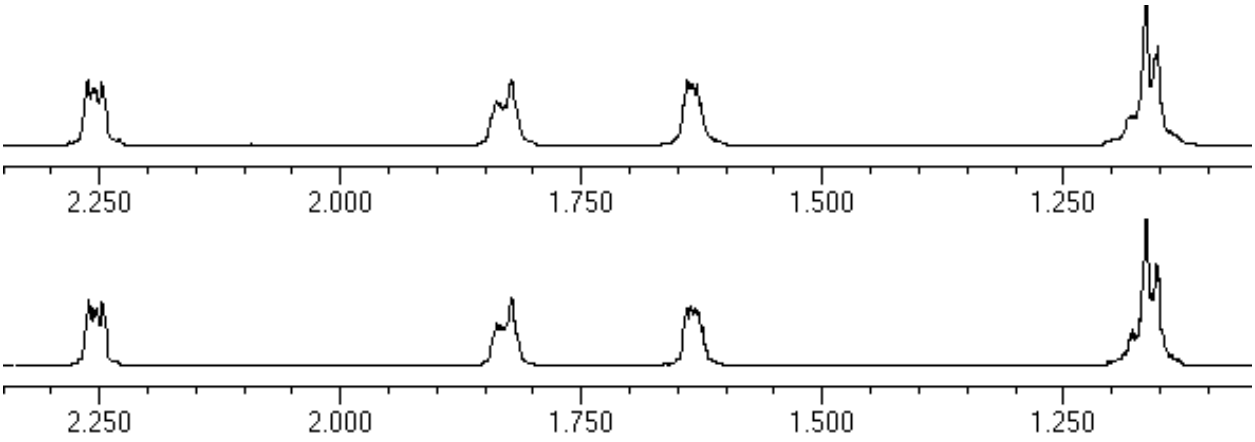

Figure 3: The experimental and simulated ^{1}H NMR spectra of *trans*-1,2-CDCA in D_2O at pH = 5.49. The bottom spectrum is the computed one.

#	Nucleus	n	Shift	Width	J[1]	J[2]	J[3]	J[4]	J[5]	J[6]	J[7]	J[8]	J[9]
1	1H	1	2.254										
			A	-									
2	1H	1	1.828		3.26								
			B	-	AB								
3	1H	1	1.168		11.32	-12.09							
			C	-	AC	BC							
4	1H	1	1.634		-0.34	3.35	3.33						
			D	-	AD	BD	CD						
5	1H	1	1.156		0.06	3.22	12.78	-12.80					
			E	-	AE	BE	CE	DE					
6	1H	1	2.254		9.30	-0.59	0.00	-0.02	-0.15				
			F	-	AF	AG	AH	AI	AJ				
7	1H	1	1.828		-0.59	0.36	-0.04	1.01	-0.56	3.26			
			G	-	AG	BG	BH	BI	BJ	AB			
8	1H	1	1.168		0.00	-0.04	-0.16	-0.48	0.00	11.32	-12.09		
			H	-	AH	BH	CH	CI	CJ	AC	BC		
9	1H	1	1.634		-0.02	1.01	-0.48	3.11	2.30	-0.34	3.35	3.33	
			I	-	AI	BI	CI	DI	DJ	AD	BD	CD	
10	1H	1	1.156		-0.15	-0.56	0.00	2.30	12.43	0.06	3.22	12.78	-12.80
			J	-	AJ	BJ	CJ	DJ	EJ	AE	BE	CE	DE

Figure 4: The chemicals shifts and coupling constants for the computed ^{1}H NMR spectrum of *trans*-1,2-CDCA in D_2O at pH = 5.49.

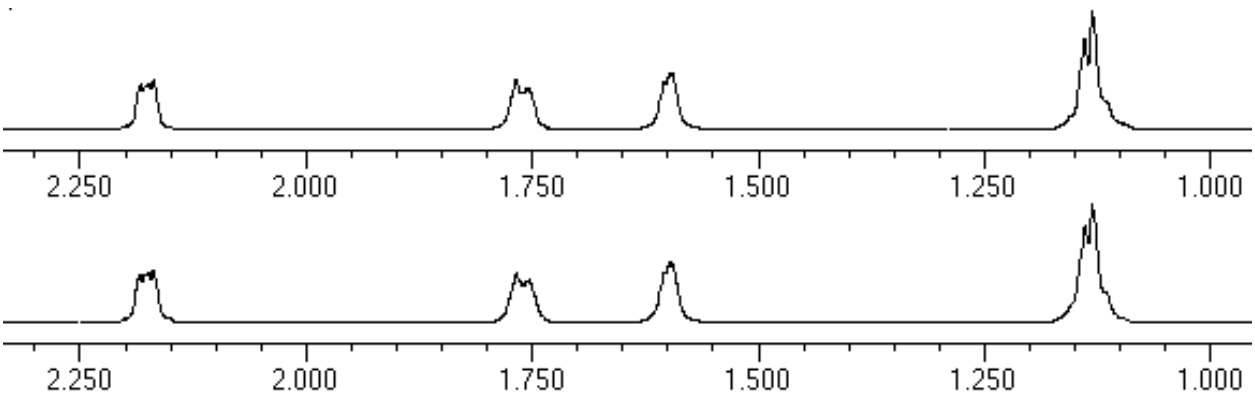

Figure 5: The experimental and simulated ^{1}H NMR spectra of *trans*-1,2-CDCA in D_2O at pH = 9.56. The bottom spectrum is the computed one.

#	Nucleus	n	Shift	Width	J[1]	J[2]	J[3]	J[4]	J[5]	J[6]	J[7]	J[8]	J[9]
1	1H	1	2.176										
			A	-									
2	1H	1	1.761		4.10								
			B	-	AB								
3	1H	1	1.129		12.40	-13.15							
			C	-	AC	BC							
4	1H	1	1.598		0.00	3.20	3.37						
			D	-	AD	BD	CD						
5	1H	1	1.135		0.00	3.60	12.64	-13.05					
			E	-	AE	BE	CE	DE					
6	1H	1	2.176		10.40	-0.86	0.00	0.00	0.00				
			F	-	AF	AG	AH	AI	AJ				
7	1H	1	1.761		-0.86	1.00	0.00	1.68	-0.30	4.10			
			G	-	AG	BG	BH	BI	BJ	AB			
8	1H	1	1.129		0.00	0.00	0.00	-0.42	0.05	12.40	-13.15		
			H	-	AH	BH	CH	CI	CJ	AC	BC		
9	1H	1	1.598		0.00	1.68	-0.42	3.14	3.43	0.00	3.20	3.37	
			I	-	AI	BI	CI	DI	DJ	AD	BD	CD	
10	1H	1	1.135		0.00	-0.30	0.05	3.43	13.14	0.00	3.60	12.64	-13.05
			J	-	AJ	BJ	CJ	DJ	EJ	AE	BE	CE	DE

Figure 6: The chemicals shifts and coupling constants for the computed ^{1}H NMR spectrum of *trans*-1,2-CDCA in D_2O at pH = 9.56.

Spectra of cis-1,3-CDCA in D_2O

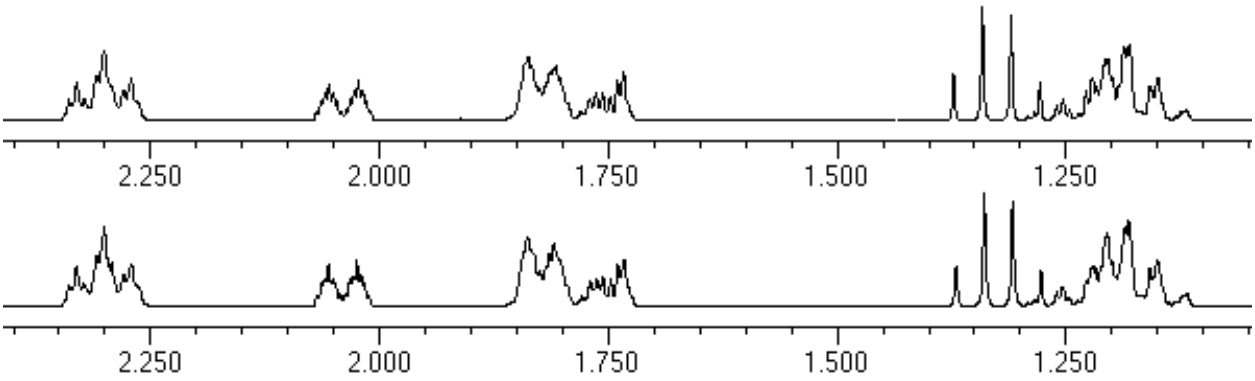

Figure 7: The experimental and simulated ^1H NMR spectra of *cis*-1,3-CDCA in D_2O at pH = 2.38. The bottom spectrum is the computed one.

#	Nucleus	n	Shift	Width	J[1]	J[2]	J[3]	J[4]	J[5]	J[6]	J[7]	J[8]	J[9]
1	1H	1	2.300										
			A16	-									
2	1H	1	2.040		3.21								
			B14	-	AB								
3	1H	1	1.324		12.39	-12.40							
			C13	-	AC	BC							
4	1H	1	1.823		3.52	2.00	0.00						
			D4	-	AD	BD	CD						
5	1H	1	1.173		12.36	0.00	0.00	-13.02					
			E5	-	AE	BE	CE	DE					
6	1H	1	1.747		0.00	0.00	0.00	3.11	3.69				
			F7	-	AF	BF	CF	DF	EF				
7	1H	1	1.230		0.00	0.00	0.00	3.52	13.20	-13.45			
			G8	-	AG	BG	CG	DG	EG	FG			
8	1H	1	2.300		0.00	3.21	12.39	0.00	0.00	0.00	0.00		
			A18	-	AAp	AB	AC	ADp	AEp	AF	AG		
9	1H	1	1.823		0.00	2.00	0.00	0.00	0.00	3.11	3.52	3.52	
			D10	-	ADp	BD	CD	DDp	EDp	DF	DG	AD	
10	1H	1	1.173		0.00	0.00	0.00	0.00	0.00	3.69	13.20	12.36	-13.02
			E11	-	AEp	BE	CE	DEp	EEp	EF	EG	AE	DE

Figure 8: The chemicals shifts and coupling constants for the computed ^{1}H NMR spectrum of *cis*-1,3-CDCA in D_2O at pH = 2.38.

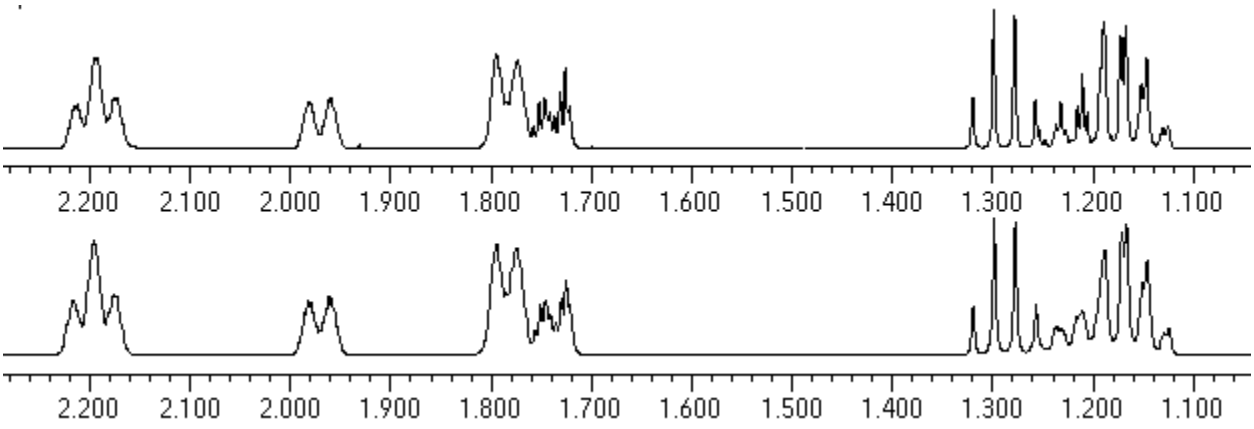

Figure 9: The experimental and simulated ^{1}H NMR spectra of *cis*-1,3-CDCA in D_2O at pH = 4.45. The bottom spectrum is the computed one.

#	Nucleus	n	Shift	Width	J[1]	J[2]	J[3]	J[4]	J[5]	J[6]	J[7]	J[8]	J[9]
1	1H	1	2.195										
			A16	-									
2	1H	1	1.971		3.58								
			B14	-	AB								
3	1H	1	1.288		12.57	-12.54							
			C13	-	AC	BC							
4	1H	1	1.784		3.62	2.00	0.00						
			D4	-	AD	BD	CD						
5	1H	1	1.160		12.68	0.00	0.00	-12.85					
			E5	-	AE	BE	CE	DE					
6	1H	1	1.736		-0.44	0.00	0.00	2.80	3.56				
			F7	-	AF	BF	CF	DF	EF				
7	1H	1	1.219		1.54	-1.53	-0.27	3.70	13.20	-13.34			
			G8	-	AG	BG	CG	DG	EG	FG			
8	1H	1	2.195		0.08	3.58	12.57	0.00	-0.03	-0.44	1.54		
			A18	-	AAp	AB	AC	ADp	AEp	AF	AG		
9	1H	1	1.784		0.00	2.00	0.00	1.12	0.00	2.80	3.70	3.62	
			D10	-	ADp	BD	CD	DDp	EDp	DF	DG	AD	
10	1H	1	1.160		-0.03	0.00	0.00	-0.01	0.02	3.56	13.20	12.68	-12.85
			E11	-	AEp	BE	CE	DEp	EEp	EF	EG	AE	DE

Figure 10: The chemicals shifts and coupling constants for the computed ^{1}H NMR spectrum of *cis*-1,3-CDCA in D_2O at pH = 4.45.

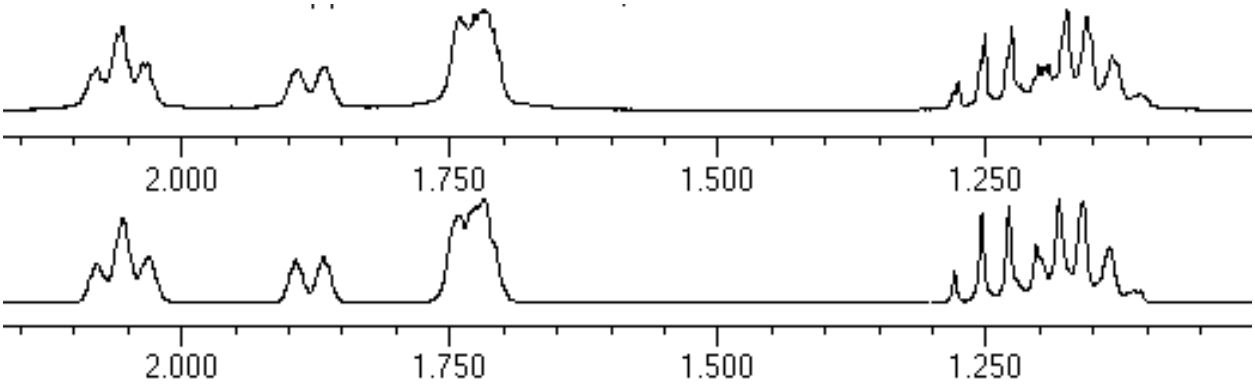

Figure 11: The experimental and simulated ^{1}H NMR spectra of *cis*-1,3-CDCA in D_2O at pH = 10.44. The bottom spectrum is the computed one.

#	Nucleus	n	Shift	Width	J[1]	J[2]	J[3]	J[4]	J[5]	J[6]	J[7]	J[8]	J[9]
1	1H	1	2.195										
			A16	-									
2	1H	1	1.971		3.58								
			B14	-	AB								
3	1H	1	1.288		12.57	-12.54							
			C13	-	AC	BC							
4	1H	1	1.784		3.62	2.00	0.00						
			D4	-	AD	BD	CD						
5	1H	1	1.160		12.68	0.00	0.00	-12.85					
			E5	-	AE	BE	CE	DE					
6	1H	1	1.736		-0.44	0.00	0.00	2.80	3.56				
			F7	-	AF	BF	CF	DF	EF				
7	1H	1	1.219		1.54	-1.53	-0.27	3.70	13.20	-13.34			
			G8	-	AG	BG	CG	DG	EG	FG			
8	1H	1	2.195		0.08	3.58	12.57	0.00	-0.03	-0.44	1.54		
			A18	-	AAp	AB	AC	ADp	AEp	AF	AG		
9	1H	1	1.784		0.00	2.00	0.00	1.12	0.00	2.80	3.70	3.62	
			D10	-	ADp	BD	CD	DDp	EDp	DF	DG	AD	
10	1H	1	1.160		-0.03	0.00	0.00	-0.01	0.02	3.56	13.20	12.68	-12.85
			E11	-	AEp	BE	CE	DEp	EEp	EF	EG	AE	DE

Figure 12: The chemicals shifts and coupling constants for the computed ^{1}H NMR spectrum of *cis*-1,3-CDCA in D_2O at pH = 10.44

Spectra of trans-1,2-CDCA in DMSO

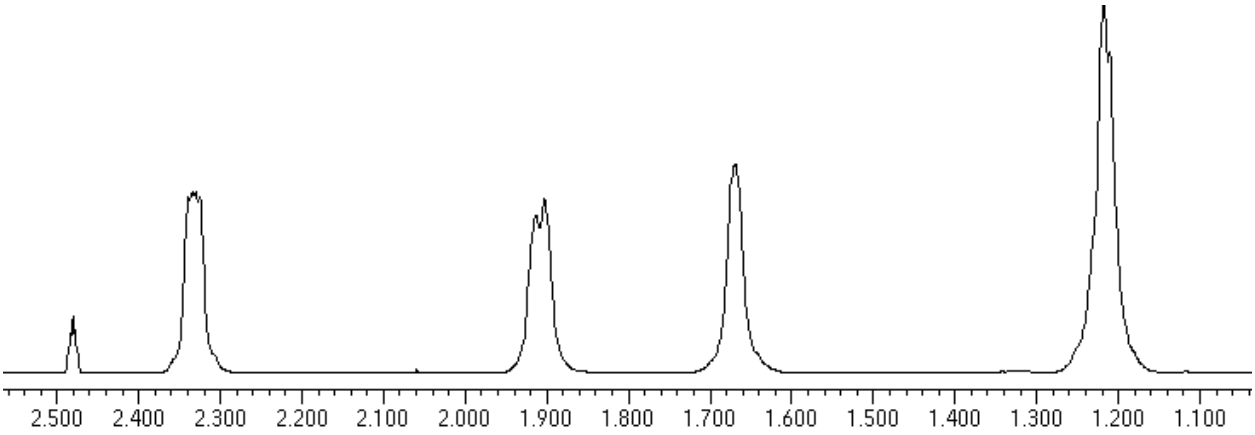

Figure 13: The ^{1}H NMR spectrum of *trans*-1,2-CDCA in DMSO.

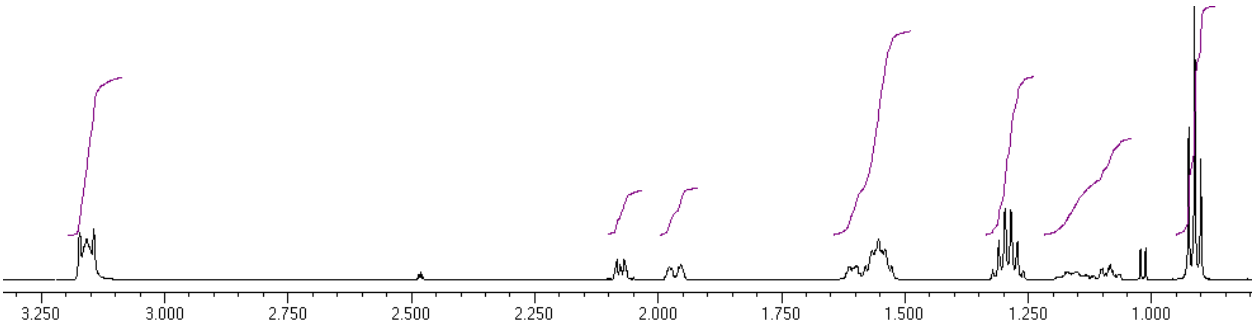

Figure 14: The ^{1}H NMR spectrum of the monoanion of *trans*-1,2-CDCA in DMSO using tetrabutylammonium as counterion.

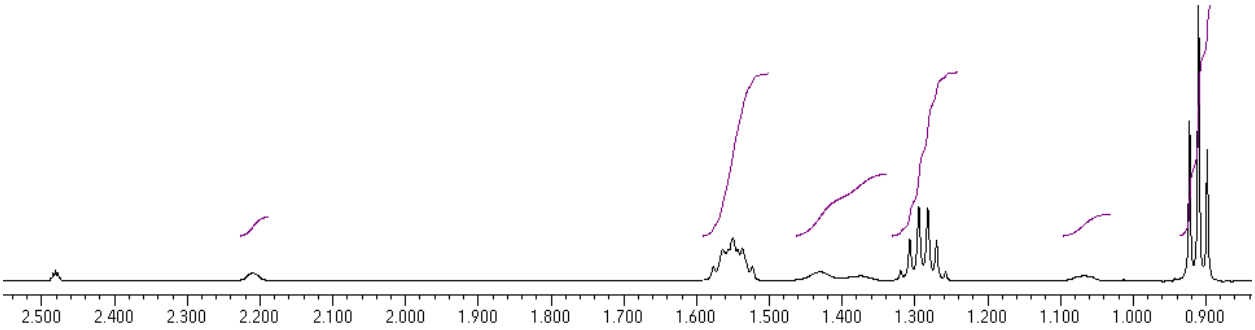

Figure 15: The ^{1}H NMR spectrum of the dianion of *trans*-1,2-CDCA in DMSO using tetrabutylammonium as counterion.

Spectra of cis-1,3-CDCA in DMSO

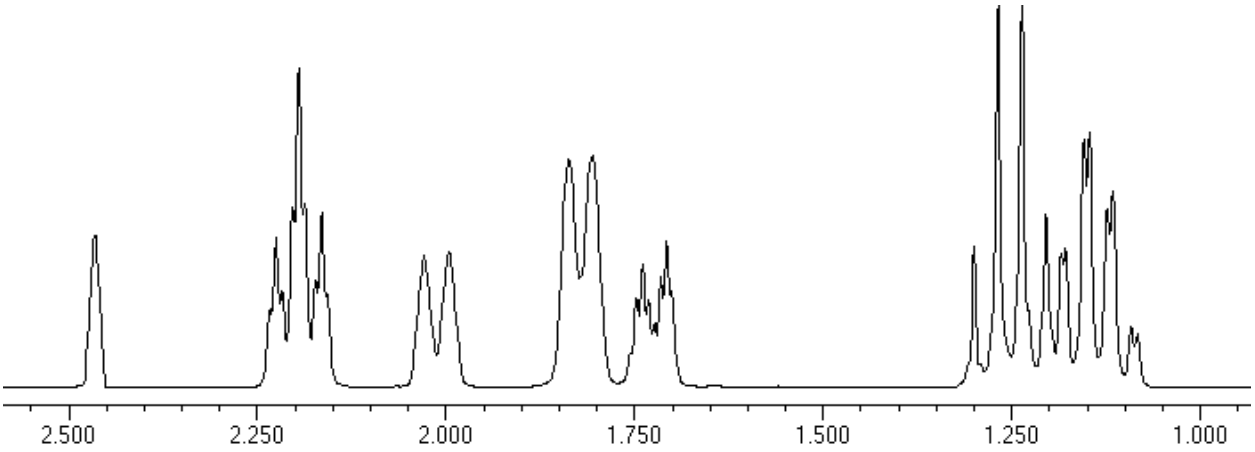

Figure 16: The ^{1}H NMR spectrum of *cis*-1,3-CDCA in DMSO.

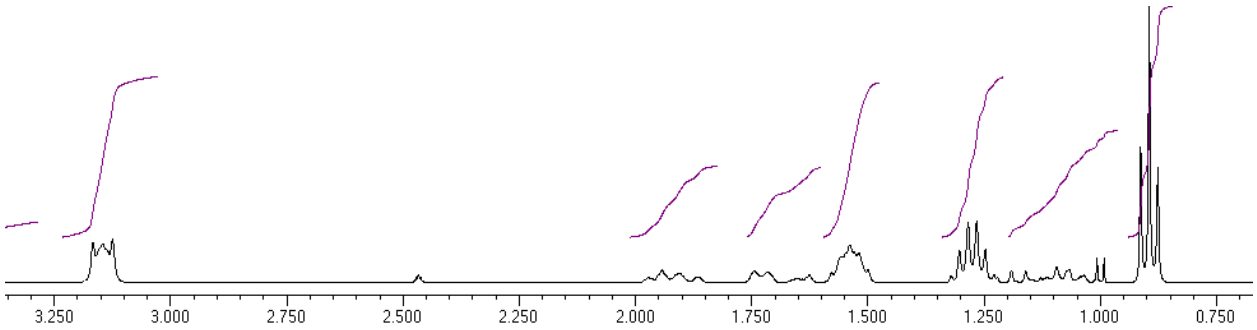

Figure 17: The ^{1}H NMR spectrum of the monoanion of *cis*-1,2-CDCA in DMSO using tetrabutylammonium as counterion.

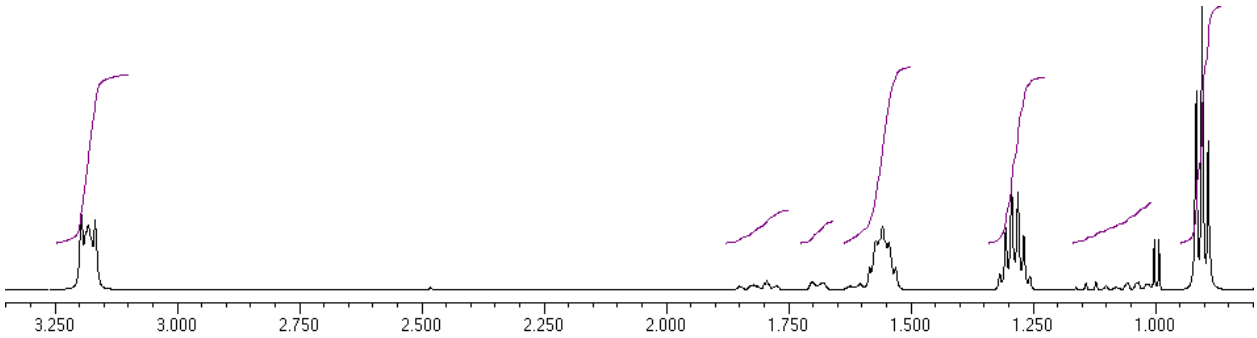

Figure 18: The ^{1}H NMR spectrum of the dianion of *cis*-1,2-CDCA in DMSO using tetrabutylammonium as counterion.

M06-2X/cc-pVTZ(-f)++ geometries (.xyz Files)

trans-1,2-CDCA in water

aaEZ

C1 -0.0046438054 0.0004696167 -0.0715749679

C2 -0.0644574382 0.0066974338 1.4555461972

C3 1.4423031154 -0.0192637846 -0.5635556388

H4 -0.5462753965 -0.8680276877 -0.4433699940

H5 -0.5178494513 0.8821902784 -0.4706452858

C6 2.2235579604 1.1774853117 -0.0187266100

H7 1.4709241081 -0.0000331679 -1.6523342390

H8 1.9209756311 -0.9531200352 -0.2562319119

C9 2.1548302034 1.3007163095 1.5082294983

H10 3.2685397793 1.1214324525 -0.3151032285

H11 1.8231574944 2.0959714779 -0.4471310072

C12 0.7261882908 1.1811483675 2.0736702907

H13 0.3517221949 -0.9241256913 1.8480009193

H14 -1.0990732405 0.0420891745 1.7964657254

C15 3.0857456711 0.3156438159 2.1819557681

H16 2.5423465839 2.2796402062 1.8033153949

O17 3.8486529674 -0.4215504308 1.6060181367

O18 3.0249228777 0.3656038923 3.5163941010

C19 -0.0261739482 2.4750586266 1.8803431297

H20 0.7712301709 1.0361169805 3.1530287524

O21 -1.2017708517 2.5672546624 2.5157294993

O22 0.3446761618 3.4047499223 1.2086369164

H23 3.6796489131 -0.2487381458 3.8901812612

H24 -1.3870217874 1.7965004365 3.0728330737

aaZZ

C1 -0.0208056760 0.0150982358 -0.0993638375

C2 -0.1704049142 -0.1348462276 2.4420603045

C3 2.0868265186 0.0854981446 1.3160526014

C4 1.3182016901 -0.4843552675 2.5105101814

C5 1.4772349777 -0.3329230566 -0.0260826576

C6 -0.7927461739 -0.5468322534 1.1055758040

H7 -0.3001826290 0.9418680987 2.5943437150

H8 2.0733126404 1.1757531217 1.3592704336

H9 1.4415072309 -1.5704035111 2.5449635772

H10 -0.7872293606 -1.6367544422 1.0196429734

H11 -0.7058906277 -0.6281161741 3.2519045653

H12 3.1310073129 -0.2179090098 1.3495751068

H13 1.7479044712 -0.0943942462 3.4323444492

H14 -1.8357322138 -0.2418834181 1.0525693851

H15 -0.4520416834 -0.3959394333 -1.0158148983

H16 1.9874960217 0.1976186990 -0.8343738060

C17 -0.1739558827 1.5157422694 -0.2752049177

C18 1.7646577585 -1.7887410626 -0.3218277390

O19 2.6059725498 -2.4454870932 0.2446266130

O20 0.7069511619 2.2547484042 -0.6469781616

O21 1.0454926103 -2.2916546239 -1.3289204401

H22 1.3398599106 -3.2039284746 -1.5000200528

O23 -1.4064971168 1.9627010138 -0.0299630080

H24 -1.4406737393 2.9181369866 -0.2182240149

eeZZ

C1 0.0071629524 0.0122669446 -0.0046041816

C2 0.0076334773 0.0242763884 2.5195403227

C3 2.2045423217 -0.0615457342 1.2722738225

C4 1.4418585862 -0.5037664590 2.5220777886

C5 1.4515368352 -0.4875539197 -0.0004990906

C6 -0.7500898776 -0.4152725094 1.2655303617

H7 0.0213917373 1.1169075423 2.5674676439

H8 2.3299134080 1.0245523379 1.2774735279

H9 1.4268318258 -1.5966574173 2.5660730309

H10 1.4599169616 -1.5782902057 -0.0511570316

H11 -0.8733385414 -1.5014661491 1.2670002244

H12 -0.0021737867 1.1022559031 -0.0594752241

H13 -0.5226824978 -0.3212152614 3.4072451563

H14 3.2004086499 -0.5016035098 1.2585215116

H15 1.9687599915 -0.1614847315 3.4132650609

H16 -1.7467759131 0.0232439401 1.2496747585

C17 2.1510891117 0.0219256227 -1.2364304035

O18 1.7586390737 0.9498756639 -1.9059861981

O19 3.2686114348 -0.6398784146 -1.5373777566

H20 3.6665998911 -0.2439521846 -2.3326210350

C21 -0.6891206467 -0.5078726237 -1.2375794403

O22 -0.3406779688 -1.4895439273 -1.8528547753

O23 -1.7550129794 0.2062801189 -1.5993493455

H24 -2.1588244037 -0.2027546903 -2.3847463614

eeEZ

C1 0.0956958305 0.0810185367 -0.0527753696

C2 -0.1156990821 0.0590892223 2.4574664279

C3 2.1710142517 -0.0281225323 1.3483118022

C4 1.3343226295 -0.4168701049 2.5687829351

C5 1.4944245263 -0.5174277532 0.0543518184

C6 -0.7607893315 -0.3806605737 1.1438399303

H7 -0.1535995817 1.1499056571 2.5222124894

H8 2.2912849214 1.0580280151 1.3015429762

H9 1.3526808519 -1.5049501573 2.6755580302

H10 1.4196719599 -1.6079590496 0.0994751469

H11 -0.8530333638 -1.4700169436 1.1060006721

H12 0.1585807326 1.1722415882 -0.0396035294

H13 -0.6979701845 -0.3248323743 3.2953523601

H14 3.1673009694 -0.4602662580 1.4177802665

H15 1.7901039145 -0.0058722630 3.4700485849

H16 -1.7682672435 0.0258866307 1.0581002288

C17 2.3850140099 -0.2567127626 -1.1358084448

O18 3.4310285833 -0.8377140920 -1.3109428028

O19 1.9416607408 0.6730306702 -1.9827689754

H20 2.5695914594 0.7563185322 -2.7226778161

C21 -0.5874978091 -0.3308752488 -1.3256608293

O22 -0.3691629261 -1.3649460257 -1.9087248709

O23 -1.5246632351 0.4981192990 -1.7971006879

H24 -1.5907773017 1.3103568345 -1.2726727289

trans-1,2-CDCA in DMSO

aaEZ

C1 0.0003822437 -0.0026508926 -0.0526845881

C2 -0.0427518368 0.0006252854 1.4755767150

C3 1.4421823750 -0.0074533977 -0.5618546209

H4 -0.5369275617 -0.8751083029 -0.4215543791

H5 -0.5261060501 0.8749892781 -0.4433745886

C6 2.2267347126 1.1853844840 -0.0118250343

H7 1.4565196979 0.0267374856 -1.6507260223

H8 1.9295296766 -0.9429125924 -0.2735755544

C9 2.1608441733 1.3035047644 1.5159355333

H10 3.2708744657 1.1268659762 -0.3110522200

H11 1.8275341370 2.1069611028 -0.4343115300

C12 0.7312325666 1.1922500636 2.0814527852

H13 0.4004074665 -0.9211516040 1.8609773919

H14 -1.0734502907 0.0097632937 1.8299127363

C15 3.0845684084 0.3078030770 2.1878431093

H16 2.5578204525 2.2782742829 1.8117514070

O17 3.8577972219 -0.4177279532 1.6082225864

O18 3.0024119902 0.3344172486 3.5214209227

C19 -0.0313905535 2.4819240136 1.8657395548

H20 0.7797969292 1.0594964767 3.1624421529

O21 -1.2148876447 2.5785092383 2.4875998729

O22 0.3406910628 3.4018405898 1.1817159603

H23 3.6540233650 -0.2852330142 3.8915113485

H24 -1.3883542245 1.8240607564 3.0694452552

aaZZ

C1 -0.0064435184 0.0168347133 -0.0972237651

C2 -0.1594807203 -0.1184784860 2.4407899101

C3 2.1058111670 0.0731700729 1.3207752046

C4 1.3276290961 -0.4739850670 2.5198940589

C5 1.4907472239 -0.3331331819 -0.0229794237

C6 -0.7762976005 -0.5480568712 1.1076364282

H7 -0.2857259854 0.9613642597 2.5741182360

H8 2.1171620522 1.1635442629 1.3610348300

H9 1.4453065897 -1.5598378346 2.5736717218

H10 -0.7570118606 -1.6386674763 1.0294618984

H11 -0.7000146986 -0.5947208986 3.2573575588

H12 3.1428518777 -0.2542829404 1.3570967709

H13 1.7559572884 -0.0702432843 3.4367575238

H14 -1.8221585988 -0.2550452817 1.0483236840

H15 -0.4339452782 -0.3963433090 -1.0137545960

H16 2.0059051077 0.2003091213 -0.8259380723

C17 -0.1743108555 1.5155936824 -0.2656967181

C18 1.7540826754 -1.7920086270 -0.3310264300

O19 2.5554860333 -2.4814217601 0.2548700067

O20 0.7096146452 2.2734572781 -0.5903528242

O21 1.0516254959 -2.2543649691 -1.3692508489

H22 1.3216147769 -3.1724899743 -1.5438608211

O23 -1.4268727782 1.9324103300 -0.0699009822

H24 -1.4715482697 2.8882756104 -0.2489140949

eeEZ

C1 0.0685630420 0.0800748473 -0.0520832734

C2 -0.1320384180 0.0535124747 2.4689162943

C3 2.1467039823 -0.0439370409 1.3674526207

C4 1.3061995904 -0.4534808375 2.5765620270

C5 1.4775545520 -0.5011397219 0.0593107544

C6 -0.7835293343 -0.3700656714 1.1525633307

H7 -0.1448710359 1.1445003118 2.5415076380

H8 2.2695059210 1.0427317479 1.3479895175

H9 1.3024843680 -1.5442883454 2.6565653540

H10 1.4101224549 -1.5929108586 0.0741216679

H11 -0.8895347227 -1.4579830703 1.1179957168

H12 0.1222318861 1.1716591433 -0.0566430396

H13 -0.7237400432 -0.3220366009 3.3042177005

H14 3.1428261795 -0.4784874014 1.4285649532

H15 1.7681408998 -0.0740397850 3.4885042064

H16 -1.7867588568 0.0490373962 1.0724578943

C17 2.3748847188 -0.1946036267 -1.1178150678

O18 3.4755698063 -0.6764626006 -1.2508016880

O19 1.8574785479 0.6594372600 -2.0025796897

H20 2.4812511801 0.7745040565 -2.7410452789

C21 -0.6086307057 -0.3718125438 -1.3223634466

O22 -0.4269233706 -1.4502154928 -1.8319535585

O23 -1.4956179722 0.4659316954 -1.8709580735

H24 -1.5370178692 1.3107959238 -1.3997985582

eeZZ

C1 0.0091768525 0.0111260761 -0.0014877487

C2 -0.0042828393 0.0014082571 2.5222870973

C3 2.1955273141 -0.0326675220 1.2711592106

C4 1.4471625890 -0.4780421420 2.5281760195

C5 1.4516756419 -0.4922687076 0.0039337332

C6 -0.7434371438 -0.4473812628 1.2609591059

H7 -0.0282424923 1.0934645873 2.5799406047

H8 2.2910457631 1.0568171996 1.2585969973

H9 1.4705008066 -1.5698807446 2.5891065210

H10 1.4603596459 -1.5843856126 -0.0237857294

H11 -0.8377657762 -1.5369813853 1.2495775346

H12 0.0013781246 1.1032445280 -0.0304857319

H13 -0.5251632392 -0.3701899734 3.4054748177

H14 3.2043331041 -0.4430738568 1.2640313711

H15 1.9618424975 -0.1039485333 3.4139389931

H16 -1.7525647559 -0.0381484580 1.2460611857

C17 2.1737853312 -0.0117023733 -1.2278374945

O18 1.8148489030 0.9229845103 -1.9078073078

O19 3.2806505638 -0.7050933872 -1.4961301657

H20 3.7063002500 -0.3232672254 -2.2824095507

C21 -0.7051637036 -0.4700081602 -1.2373990744

O22 -0.3530341229 -1.4165399407 -1.9042784822

O23 -1.7980954702 0.2373170044 -1.5251558391

H24 -2.2209056566 -0.1476728909 -2.3114189224

trans-1,2-CDCA monoanion in water

aaZ

C1 -0.0031907773 -0.0273975716 0.0219603137

C2 0.0241298699 0.0455920660 2.5406599775

C3 2.2356301434 -0.0340614802 1.3075346825

C4 1.4740251619 -0.4322026087 2.5737669700

C5 1.5120308708 -0.3222337649 -0.0142949919

C6 -0.6807862543 -0.5141576362 1.3088372429

H7 -0.0122035928 1.1404346012 2.5215415750

H8 2.4182625440 1.0397663977 1.3317749545

H9 1.4840900732 -1.5173081730 2.6925595937

H10 -0.6667011073 -1.6060309904 1.3427635001

H11 -0.4984067021 -0.2636117178 3.4441791491

H12 3.2112251530 -0.5191903816 1.2866980096

H13 1.9931088048 -0.0138483105 3.4355642730

H14 -1.7247490459 -0.2114148899 1.2800424357

H15 -0.4883484716 -0.5096479493 -0.8289651179

H16 1.9402862300 0.3216858621 -0.7799757858

C17 -0.2616615368 1.4652940943 -0.1666029911

C18 1.6832161048 -1.7279458452 -0.5001898772

O19 1.9104533384 -2.6916993083 0.1893137137

O20 0.7108056812 2.2377999115 -0.2990490577

O21 -1.4632226476 1.8197337682 -0.1871599747

O22 1.5235092617 -1.9101819087 -1.8248261186

H23 1.4040213365 -1.0721078087 -2.2968224413

aaE

C1 -0.0031907773 -0.0273975716 0.0219603137

C2 0.0241298699 0.0455920660 2.5406599775

C3 2.2356301434 -0.0340614802 1.3075346825

C4 1.4740251619 -0.4322026087 2.5737669700

C5 1.5120308708 -0.3222337649 -0.0142949919

C6 -0.6807862543 -0.5141576362 1.3088372429

H7 -0.0122035928 1.1404346012 2.5215415750

H8 2.4182625440 1.0397663977 1.3317749545

H9 1.4840900732 -1.5173081730 2.6925595937

H10 -0.6667011073 -1.6060309904 1.3427635001

H11 -0.4984067021 -0.2636117178 3.4441791491

H12 3.2112251530 -0.5191903816 1.2866980096

H13 1.9931088048 -0.0138483105 3.4355642730

H14 -1.7247490459 -0.2114148899 1.2800424357

H15 -0.4883484716 -0.5096479493 -0.8289651179

H16 1.9402862300 0.3216858621 -0.7799757858

C17 -0.2616615368 1.4652940943 -0.1666029911

C18 1.6832161048 -1.7279458452 -0.5001898772

O19 1.9104533384 -2.6916993083 0.1893137137

O20 0.7108056812 2.2377999115 -0.2990490577

O21 -1.4632226476 1.8197337682 -0.1871599747

O22 1.5235092617 -1.9101819087 -1.8248261186

H23 1.4040213365 -1.0721078087 -2.2968224413

eeZ

C1 -0.0495855713 0.0132701828 0.0361905012

C2 0.0581937187 -0.0592327282 2.5596642450

C3 2.1879584373 0.0443133965 1.2420771092

C4 1.5251433705 -0.4850491990 2.5061535196

C5 1.4389092239 -0.3980974224 -0.0212680780

C6 -0.7007095087 -0.5115054778 1.3125150229

H7 0.0036698643 1.0301438294 2.6443277089

H8 2.2167826867 1.1356568692 1.2675262904

H9 1.5933206218 -1.5767168486 2.5228141700

H10 1.5008388915 -1.4837758835 -0.1081020866

H11 -0.7130784300 -1.6028029917 1.2684037212

H12 -0.0940163585 1.1031181103 -0.0072007558

H13 -0.4226469110 -0.4688497585 3.4475789449

H14 3.2242177522 -0.2940943460 1.1716587372

H15 2.0592784226 -0.1220461354 3.3846429085

H16 -1.7405651667 -0.1866738849 1.3522977335

C17 2.1226458764 0.2073636033 -1.2317855260

C18 -0.7609454418 -0.5158860201 -1.1872469454

O19 -1.4513288232 -1.5095964326 -1.2095706045

O20 2.6571995437 -0.5734076935 -2.0535583647

O21 2.1403098144 1.4546005633 -1.3221490841

O22 -0.5416883310 0.2032940340 -2.2920523561

H23 -0.9868184608 -0.2224437853 -3.0459708420

eeE (H-bonded)

C1 0.0057522633 -0.0220892955 -0.0048847472

C2 -0.0016598152 -0.0064895717 2.5417283166

C3 2.1742341578 -0.0106915616 1.2864459599

C4 1.4553132218 -0.4623402394 2.5515435442

C5 1.4687495687 -0.5082322334 0.0282531251

C6 -0.7162710384 -0.4724236457 1.2793286390

H7 -0.0420759760 1.0856322007 2.5936057662

H8 2.2151274084 1.0806650747 1.2509800954

H9 1.4983138685 -1.5533240024 2.6217120964

H10 1.4542522251 -1.6035959909 0.0199873932

H11 -0.7814729258 -1.5657626003 1.2716776635

H12 -0.0140085050 1.0707186503 -0.0521209099

H13 -0.5253491343 -0.3850424528 3.4198724881

H14 3.2062605038 -0.3588690532 1.2802944333

H15 1.9715672601 -0.0708798018 3.4276422981

H16 -1.7363735819 -0.0955569904 1.2498730650

C17 2.2610824281 -0.1061056625 -1.1997505937

C18 -0.8411883003 -0.5285394541 -1.1692309388

O19 -1.9655376121 -0.0311497840 -1.3153952821

O20 1.8868133943 -0.6506046583 -2.3393633998

O21 3.2126858739 0.6498830704 -1.1662047342

O22 -0.3808005816 -1.4640389772 -1.9049429848

H23 0.9725917618 -1.1341915451 -2.1983278947

trans-1,2-CDCA monoanion in DMSO

aaE

C1 0.0138694628 -0.0000883780 0.0005070219

C2 0.0885557088 -0.0126266345 2.5279226686

C3 2.2527164560 0.0057448075 1.2055449383

C4 1.5584165241 -0.4334547776 2.4973192977

C5 1.4975644600 -0.4027350405 -0.0624240144

C6 -0.6549162621 -0.5001256937 1.2838858257

H7 0.0174609333 1.0778798172 2.5833598485

H8 2.3301174145 1.0939747600 1.1908536598

H9 1.6269832254 -1.5188273461 2.6014539533

H10 -0.6811265632 -1.5942381206 1.2770852335

H11 -0.3928571931 -0.4002409864 3.4253934618

H12 3.2680710574 -0.3858609646 1.1701622703

H13 2.0870087868 -0.0024095239 3.3472456623

H14 -1.6863216685 -0.1590760026 1.2962555687

H15 -0.5036844579 -0.4236641258 -0.8622342494

H16 1.9328753862 0.1169781291 -0.9169889315

C17 -0.1509646214 1.5240322267 -0.1664512741

C18 1.6649016289 -1.8667645633 -0.3775648667

O19 2.3404439087 -2.6487760346 0.2525429282

O20 0.7829135029 2.1607658855 -0.7059691313

O21 -1.2360919643 2.0167144335 0.2200153857

O22 1.0079529432 -2.2445680569 -1.4832609580

H23 1.190570631 -3.184470328 -1.6491785430

aaE

C1 0.0001731654 0.0061082522 -0.0139196710

C2 0.0015057377 -0.0102239200 2.5051832506

C3 2.2206343949 -0.0080171741 1.2751142183

C4 1.4675149800 -0.4398875986 2.5371468122

C5 1.5082755694 -0.3244038856 -0.0471309730

C6 -0.6845342548 -0.5338775557 1.2452751341

H7 -0.0691067655 1.0821440432 2.5271345770

H8 2.3590724970 1.0731037773 1.2985608145

H9 1.5189292531 -1.5242052708 2.6494882367

H10 -0.6576943309 -1.6267654485 1.2404939506

H11 -0.5158559168 -0.3721431350 3.3925885278

H12 3.2145581093 -0.4556648148 1.2607188821

H13 1.9668180682 -0.0068574371 3.4041801053

H14 -1.7304975560 -0.2393340613 1.2206185638

H15 -0.4839641528 -0.4314669508 -0.8909299381

H16 1.9524769933 0.2886057464 -0.8303522948

C17 -0.2404494895 1.5220864259 -0.1518954803

C18 1.6722806159 -1.7569593334 -0.4732901514

O19 1.9317016493 -2.6802709873 0.2591324835

O20 0.7322154431 2.2583856475 -0.4278349565

O21 -1.4234638230 1.9028143813 0.0034060873

O22 1.4798473365 -2.0139156502 -1.7817031386

H23 1.3431540065 -1.2020709131 -2.2920325273

eeZ

C1 0.0172429137 0.0745317109 -0.0119497477

C2 -0.0340148737 -0.0144923572 2.5135074696

C3 2.1734903287 0.0058411927 1.2983680744

C4 1.4205757150 -0.4851799921 2.5306030966

C5 1.4616805716 -0.4149429310 0.0120068804

C6 -0.7471714997 -0.4268575194 1.2245571588

H7 -0.0626530430 1.0751500523 2.6062556488

H8 2.2587020825 1.0973951346 1.3223531111

H9 1.4467632774 -1.5788180226 2.5479957465

H10 1.4558353627 -1.5082003687 -0.0350876229

H11 -0.8117750096 -1.5165324270 1.1698962421

H12 0.0024414135 1.1647249104 -0.0313180653

H13 -0.5706792554 -0.4151864821 3.3737183073

H14 3.1876844166 -0.3868174642 1.2782972608

H15 1.9176036931 -0.1444444780 3.4397567195

H16 -1.7673726815 -0.0424409381 1.2137458685

C17 2.2285437108 0.0570373598 -1.2219324170

C18 -0.6690798503 -0.4132478542 -1.2594454509

O19 -0.5503090255 -1.5312026628 -1.7112384474

O20 3.4366316650 -0.2725183512 -1.2981683455

O21 1.6000598273 0.7295432354 -2.0723557550

O22 -1.5073497908 0.4746815070 -1.8024385535

H23 -1.9301336432 0.0645099015 -2.5754825785

eeE (H-bonded)

C1 0.0030347923 -0.0296416068 -0.0062399676

C2 -0.0003574561 0.0039574772 2.5443674093

C3 2.1737397534 -0.0200918045 1.2862026346

C4 1.4527790808 -0.4624650748 2.5544525579

C5 1.4689605510 -0.5108828101 0.0226736057

C6 -0.7162924765 -0.4675490494 1.2846484116

H7 -0.0331096690 1.0967646591 2.5904160564

H8 2.2236215598 1.0707576761 1.2522582074

H9 1.4867618638 -1.5533648739 2.6316319643

H10 1.4555996921 -1.6060382874 0.0101593442

H11 -0.7857522410 -1.5606826091 1.2884514321

H12 -0.0188807130 1.0630428521 -0.0589144378

H13 -0.5260813001 -0.3647687174 3.4258473229

H14 3.2033074989 -0.3747125128 1.2835096384

H15 1.9733965486 -0.0710799710 3.4284564284

H16 -1.7354257390 -0.0885999664 1.2529275757

C17 2.2678881205 -0.0992359013 -1.2053225174

C18 -0.8483914367 -0.5423867140 -1.1695792593

O19 -1.9843388882 -0.0659882118 -1.2936155952

O20 1.8987114067 -0.6295553146 -2.3531741515

O21 3.2218790569 0.6534534568 -1.1526930650

O22 -0.3722698660 -1.4564883015 -1.9223474509

H23 0.9850116355 -1.1106691143 -2.2147965454

trans-1,2-CDCA Dianion in water

aa

C1 -0.0026345386 -0.0041515497 0.0067823412

C2 0.0017678309 -0.0027115585 2.5464654688

C3 2.1862022057 -0.0007288662 1.2709650557

C4 1.4644728791 -0.4469788851 2.5435791760

C5 1.4564037617 -0.4573908859 0.0094953638

C6 -0.7255920840 -0.4497004651 1.2772265263

H7 -0.0482025280 1.0860050372 2.6228622536

H8 2.2568618388 1.0895542776 1.2514617697

H9 1.5131591845 -1.5361557626 2.6194964550

H10 -0.7982897511 -1.5407569990 1.2649257625

H11 -0.5085659718 -0.4016915315 3.4224011201

H12 3.2033807416 -0.3826016768 1.2596435206

H13 1.9797953517 -0.0512051639 3.4178979006

H14 -1.7425941231 -0.0670217345 1.2697997263

H15 -0.4919139614 -0.4610219103 -0.8532099124

H16 1.9427063541 -0.0221093737 -0.8636428158

C17 -0.0993929530 1.4934149802 -0.2598529365

C18 1.5526043923 -1.9553556788 -0.2167155870

O19 2.4868688334 -2.5850790892 0.3328616056

O20 0.7232954714 1.9895113079 -1.0690073205

O21 -1.0162595097 2.1391662074 0.3013222072

O22 0.7112094511 -2.4860022297 -0.9827402255

ee

C1 -0.0036447545 0.0008669097 0.0136264368

C2 0.0032313887 0.0002982433 2.5164583659

C3 2.1879120204 0.0032875845 1.2442119106

C4 1.4677437711 -0.4414288017 2.5143697404

C5 1.4279815241 -0.4946555937 0.0155678099

C6 -0.7379356584 -0.4729421887 1.2670329867

H7 -0.0394761924 1.0925686907 2.5477341874

H8 2.2568913770 1.0947751671 1.2055223072

H9 1.5159099117 -1.5323864136 2.5732359839

H10 1.4307518286 -1.5844500243 0.0282829400

H11 -0.8011916652 -1.5652741525 1.2523226213

H12 -0.0052370802 1.0911084660 0.0052386981

H13 -0.4949518049 -0.3620773337 3.4150121902

H14 3.2075751736 -0.3807501790 1.2221551389

H15 1.9776764782 -0.0544929218 3.3961781735

H16 -1.7591986973 -0.0932994453 1.2572659044

C17 2.1507604367 -0.0785047063 -1.2440307829

C18 -0.7380383030 -0.4409795902 -1.2415509961

O19 -1.7362831304 0.2389096661 -1.5922099751

O20 3.1283128348 -0.7812859957 -1.6086681271

O21 1.7683403080 0.9487461795 -1.8460003948

O22 -0.3320363098 -1.4655696184 -1.8406164395

trans-1,2-CDCA Dianion in DMSO

aa

C1 0.0067396918 0.0013743948 -0.0136235545

C2 -0.0020266209 -0.0171272641 2.5234701447

C3 2.1875273954 0.0011972579 1.2520905600

C4 1.4664657585 -0.4446747884 2.5253719797

C5 1.4641667536 -0.4617490084 -0.0116545096

C6 -0.7199688915 -0.4622039526 1.2480453765

H7 -0.0657586098 1.0710427087 2.6030278069

H8 2.2494871178 1.0927021897 1.2287092160

H9 1.5301402550 -1.5328762602 2.6045915327

H10 -0.7822054624 -1.5537207197 1.2239398192

H11 -0.5122215640 -0.4250419390 3.3960726865

H12 3.2064469115 -0.3766386306 1.2453744120

H13 1.9743951454 -0.0370707700 3.3994358648

H14 -1.7387539982 -0.0841114292 1.2387892070

H15 -0.4782224048 -0.4455264060 -0.8815081982

H16 1.9518142116 -0.0147388077 -0.8779944254

C17 -0.0966991273 1.5113714249 -0.2478802880

C18 1.5675528581 -1.9716494044 -0.2461882596

O19 2.4945484067 -2.5942257444 0.3248042266

O20 0.7373783974 2.0316746010 -1.0307614837

O21 -1.0276070077 2.1327142632 0.3180145572

O22 0.7375145325 -2.4903311592 -1.0344644508

ee

C1 0.0099517492 0.0058900595 0.0182546359

C2 0.0003353680 -0.0066571824 2.5324362172

C3 2.1867564826 0.0029781168 1.2630801477

C4 1.4649191954 -0.4465140471 2.5318454661

C5 1.4445943429 -0.4876996789 0.0174688444

C6 -0.7267289264 -0.4713549143 1.2723764568

H7 -0.0465928551 1.0854120866 2.5761189166

H8 2.2470891646 1.0955660515 1.2311804578

H9 1.5120782485 -1.5380116581 2.5889731237

H10 1.4448919445 -1.5778524654 0.0207342627

H11 -0.7864354501 -1.5641916861 1.2533718646

H12 0.0098796397 1.0960639892 0.0108635556

H13 -0.5043022582 -0.3799251458 3.4240918760

H14 3.2097643023 -0.3725489552 1.2482116674

H15 1.9733747546 -0.0621089474 3.4166586015

H16 -1.7498201420 -0.0963142514 1.2573489141

C17 2.1972907368 -0.0566452778 -1.2315440535

C18 -0.7489608370 -0.4365636971 -1.2234288293

O19 -1.7449085708 0.2559012673 -1.5569116119

O20 3.1874921626 -0.7554432029 -1.5676774374

O21 1.8189734344 0.9823369035 -1.8218473226

O22 -0.3697613784 -1.4773442221 -1.8099540000

cis-1,3-CDCA in water

aaZZ

C1 0.0131267377 0.0175787972 -0.0231241716

C2 -0.0156787679 -0.0210997244 1.5066572349

C3 1.4462080840 -0.0084133763 -0.5661012581

H4 -0.5001679707 0.9071133149 -0.3826013685

H5 -0.5173999530 -0.8452446191 -0.4329980926

C6 0.7781500346 -1.2014142375 2.0775386857

H7 -1.0474820350 -0.0807032816 1.8529010680

H8 0.3868110252 0.9142232957 1.8964301636

C9 2.2019243629 -1.3193891363 1.5145994905

H10 0.8285686090 -1.1215801373 3.1629455894

H11 0.2576390987 -2.1369062723 1.8561759108

C12 2.2226376204 -1.2174875043 -0.0270858434

H13 3.2460881265 -1.2226882405 -0.3945547191

H14 1.7434129379 -2.1149004158 -0.4199997581

C15 2.1384399208 1.3235540643 -0.3500469983

H16 1.4172420115 -0.0981942174 -1.6564627707

C17 3.1292212199 -0.2911511158 2.1180839742

H18 2.6201886424 -2.2905199810 1.7791393765

O19 2.7771757959 0.7259055072 2.6686433720

O20 4.4213446719 -0.6050556991 1.9832635567

O21 1.5655236669 2.3696550105 -0.1560213723

O22 3.4698782164 1.2620134062 -0.4522491319

H23 3.8358946141 2.1594525884 -0.3619365897

H24 4.9642461147 0.1031974157 2.3714368092

eeEZ

C1 -0.0833195728 -0.0914163443 -0.0320274892

C2 -0.1525128310 -0.1538643000 1.4960555415

C3 1.3660371781 0.0261686771 -0.4962887606

H4 -0.6594708143 0.7533722533 -0.4084176022

H5 -0.5185654339 -0.9951317858 -0.4649469118

C6 0.7178220787 -1.2788173443 2.0605535285

H7 -1.1852224132 -0.2883963891 1.8148935470

H8 0.1838185695 0.8009871272 1.9103361695

C9 2.1529112652 -1.1357500821 1.5618884239

H10 0.3290343100 -2.2509265444 1.7489977807

H11 0.7042088953 -1.2636366317 3.1497667820

C12 2.2036927116 -1.1544172609 0.0242415051

H13 1.7916790814 -2.0972716614 -0.3490502979

H14 3.2317965418 -1.0854007190 -0.3303288005

C15 1.4885850608 0.0878300126 -1.9947858869

H16 1.8084787512 0.9488130495 -0.1066831553

C17 3.0609917213 -2.2117043179 2.0907977151

H18 2.5658806816 -0.1795446618 1.8992298836

O19 2.6984079104 -3.2751253367 2.5282114201

O20 4.3758923458 -1.9555991438 2.0234543792

O21 0.6522211514 -0.2913969620 -2.7764665912

O22 2.6442329357 0.5726525718 -2.4705444930

H23 3.2243323958 0.8918218057 -1.7632742236

H24 4.5552255400 -1.0608449858 1.6972744616

eeZZ

C1 -0.5615411376 -0.1796199089 -1.1986774526

C2 0.5247253191 0.9375945028 0.8024862255

C3 -1.5107063691 -0.5227052988 1.1112363117

C4 -0.2045756192 -0.0405924530 1.7427850428

C5 -1.2874508701 -1.1583559797 -0.2618529165

C6 0.7345413673 0.3280996974 -0.5783094839

H7 -1.9932230604 -1.2426447342 1.7731933383

H8 -0.3990733239 0.4403778248 2.6998581260

H9 -2.2392530451 -1.4567082810 -0.6967787970

H10 1.2074581509 1.0527694445 -1.2375701571

H11 -0.0631756057 1.8573416736 0.7337110144

H12 0.4467193962 -0.8978315123 1.9365755702

H13 1.4288581782 -0.5084099213 -0.4869459400

H14 -1.2356061236 0.6582168798 -1.4087876050

H15 -0.6827059821 -2.0637745663 -0.1540392580

C16 -0.2531545498 -0.8020230104 -2.5386470741

C17 1.8621239204 1.3134752278 1.3865450172

O18 2.9312746311 0.9475151479 0.9555462808

O19 0.8440637233 -0.8333338592 -3.0463089834

O20 -1.3176647856 -1.3279018118 -3.1509936511

H21 -1.0399749310 -1.6949447219 -4.0094587504

O22 1.7764875920 2.0953922500 2.4671920679

H23 2.6726278041 2.2748384787 2.8024464017

H24 -2.2004436456 0.3204384216 1.0132800959

cis-1,3-CDCA in DMSO

aaZZ

C1 -0.0031949854 -0.0058539974 -0.0061558046

C2 -0.0066980141 0.0015083780 1.5241543840

C3 1.4216029405 0.0043713509 -0.5690635713

H4 -0.5561062662 0.8512471240 -0.3848394963

H5 -0.5058875857 -0.9010315910 -0.3805992248

C6 0.8341387275 -1.1339105104 2.1173659181

H7 -1.0303144946 -0.0816696705 1.8894070764

H8 0.3711532668 0.9612763682 1.8777428887

C9 2.2504910372 -1.2303580359 1.5324851885

H10 0.9005130712 -1.0156009767 3.1981942612

H11 0.3382372809 -2.0913217774 1.9377837205

C12 2.2480676928 -1.1627550005 -0.0111532186

H13 3.2675764669 -1.1345245941 -0.3879243409

H14 1.8012113165 -2.0865016711 -0.3802031756

C15 2.0738801718 1.3637668334 -0.3982506943

H16 1.3806181272 -0.1146995436 -1.6557908044

C17 3.1713347724 -0.1728414444 2.0940661660

H18 2.6931355325 -2.1859285992 1.8111735697

O19 2.8133945321 0.8540053741 2.6227499532

O20 4.4638146368 -0.4785233904 1.9411482581

O21 1.4729038366 2.3933190129 -0.2024773308

O22 3.4030126715 1.3379805976 -0.5481183274

H23 3.7426015082 2.2472734415 -0.4841295625

H24 5.0016912614 0.2496119451 2.2955708358

eeEZ

C1 0.0218177978 0.0133761299 -0.0022983723

C2 0.0198251455 0.0247457173 1.5277837518

C3 1.4519424058 0.0212960372 -0.5414388117

H4 -0.5260359619 0.8692206461 -0.3962443867

H5 -0.4811673031 -0.8841253510 -0.3684045896

C6 0.8350282900 -1.1353640158 2.1004832836

H7 -1.0043363652 -0.0256789844 1.8965466151

H8 0.4359360164 0.9714828585 1.8847186257

C9 2.2572000846 -1.1217335905 1.5440688872

H10 0.3661569320 -2.0871370961 1.8421440328

H11 0.8666230594 -1.0829667157 3.1880522082

C12 2.2467009149 -1.1820267259 0.0037899356

H13 1.7708036835 -2.1117323708 -0.3221936221

H14 3.2630447451 -1.1838247397 -0.3909438981

C15 1.4818365114 -0.0110407367 -2.0515782919

H16 1.9616223038 0.9368447913 -0.2263000717

C17 3.0804490308 -2.2680422652 2.0824189837

H18 2.7602035326 -0.1967881342 1.8447115932

O19 2.6230231563 -3.2714455439 2.5692624451

O20 4.4119304855 -2.1538635764 1.9689669142

O21 0.6051738547 -0.4669693638 -2.7429041934

O22 2.5861794560 0.4684108622 -2.6411526588

H23 3.1954353159 0.8636802856 -2.0011257923

H24 4.6703280120 -1.2887148709 1.6197967624

eeZZ

C1 -0.5184818882 -0.1903738474 -1.2003058061

C2 0.5517436549 0.9186136809 0.7823901585

C3 -1.4915755256 -0.5257322958 1.1016721694

C4 -0.1872307739 -0.0414883800 1.7335034551

C5 -1.2676870512 -1.1612020869 -0.2701789757

C6 0.7932517425 0.2673402957 -0.5743633502

H7 -1.9776238130 -1.2432752811 1.7640027241

H8 -0.3863732927 0.4564707172 2.6808372630

H9 -2.2205121177 -1.4398823370 -0.7155859493

H10 1.3101780045 0.9573256802 -1.2390812148

H11 -0.0505777788 1.8232175194 0.6660515078

H12 0.4609252492 -0.8967027158 1.9460503363

H13 1.4488832073 -0.5949510311 -0.4440598992

H14 -1.1649209226 0.6723209615 -1.3878086745

H15 -0.6787711134 -2.0775365363 -0.1647249437

C16 -0.2673645833 -0.8283425283 -2.5416944849

C17 1.8567815452 1.3374675323 1.4039194290

O18 2.9443859669 0.9266615232 1.0705328315

O19 0.8245072543 -1.0778897594 -2.9979214372

O20 -1.3916655520 -1.1124988463 -3.2058376310

H21 -1.1633898471 -1.5340197747 -4.0527442469

O22 1.7064076782 2.2121772454 2.4039779295

H23 2.5788842748 2.4072485487 2.7875236683

H24 -2.1783026521 0.3191732571 0.9990209353

cis-1,3-CDCA monoanion in water

aaZ

C1 0.0311239060 -0.0236323020 0.0031212357

C2 0.0142625914 0.0975930005 2.5776272347

C3 2.2338226151 -0.0961564274 1.3172817663

C4 1.4411341503 -0.4620893064 2.5732656124

C5 1.4910060946 -0.4928127246 0.0394625388

C6 -0.7384420619 -0.3127615142 1.3032186037

H7 2.4300871395 0.9728081131 1.3116995662

H8 1.3583679464 -1.5486066370 2.6416598757

H9 1.5006403683 -1.5798875092 -0.0689872235

H10 -0.9171191861 -1.3860976956 1.3665110883

H11 -0.5263672916 -0.3491805964 3.4193661268

H12 1.9704103409 -0.1255502467 3.4617186666

H13 -1.7180904746 0.1632634132 1.2576755157

H14 -0.4874570125 -0.5242838836 -0.8106774212

H15 2.0078915509 -0.0882348574 -0.8336415245

C16 -0.0670476900 1.4607649316 -0.2577583251

C17 -0.0232434700 1.5689915368 2.9352619872

O18 0.8823994006 2.1655421595 3.4712926236

O19 -0.8782079230 1.8524331075 -1.1361686334

O20 0.6258574415 2.2274778009 0.4439934970

O21 -1.2171473024 2.1448174778 2.7482268811

H22 -1.1815926180 3.0569351335 3.0867352473

H23 3.2020569552 -0.5955904674 1.3421961953

aaE (H-bonded)

C1 -0.0709580080 0.0228703412 -0.0187725966

C2 -0.0525166706 0.0455064637 2.6242419691

C3 2.1044688421 -0.0007263314 1.2583454827

C4 1.4024192175 -0.4669654542 2.5294282715

C5 1.3581329252 -0.5457413349 0.0461025588

C6 -0.8428067970 -0.0740676776 1.3049881038

H7 2.1465963858 1.0933108767 1.2167399175

H8 1.3837497487 -1.5577014454 2.5356909468

H9 1.3130108987 -1.6343853953 0.1081122218

H10 -1.3216098520 -1.0505309163 1.3185638923

H11 -0.5666025333 -0.5639620686 3.3634915658

H12 1.9419003630 -0.1538517040 3.4215531331

H13 -1.6536560389 0.6549416302 1.2973266245

H14 -0.6269649484 -0.5298242624 -0.7737072457

H15 1.8714880698 -0.2999565605 -0.8815029135

C16 0.0331470291 1.4195087649 -0.5865292942

C17 -0.0221022691 1.4088837693 3.2854888344

O18 0.1432251685 1.4965451428 4.4933326644

O19 0.3184751670 1.5406101547 -1.7863575934

O20 -0.1492005363 2.4257372391 0.1687162600

O21 -0.1482068476 2.4874456424 2.5662146979

H22 -0.1889842083 2.3458976911 1.5052564301

H23 3.1372235514 -0.3428809265 1.2554640390

eeZ (Conformer 1)

C1 -0.0434700652 0.0002533838 0.0221126610

C2 -0.0019057891 -0.0368739838 2.5407995178

C3 2.1606188564 -0.0107491866 1.2214591220

C4 1.4603219183 0.4090529310 2.5121112290

C5 1.4057729648 0.5019133575 0.0006756198

C6 -0.7556298725 0.4451570910 1.2897826109

H7 3.1864039193 0.3610540174 1.2210759596

H8 1.9824676632 0.0116590167 3.3821578107

H9 1.8901222360 0.1829003907 -0.9213236467

H10 -1.7796625015 0.0751944596 1.2956402355

H11 -0.0745626229 -1.1270591177 2.5889927556

H12 1.4876378105 1.4976505309 2.5962806957

H13 -0.8090365399 1.5355720277 1.2999193672

H14 -0.0263906413 -1.0918051517 -0.0284897312

H15 1.3992616496 1.5971122496 0.0011015510

C16 -0.7540865618 0.4840102610 -1.2316813364

C17 -0.7058800038 0.5184629381 3.7472006079

O18 -0.2990535898 1.4295956080 4.4313490075

O19 -1.5759175099 1.4248818814 -1.1282465415

O20 -0.4433353184 -0.0795265375 -2.3105315916

O21 -1.8859163825 -0.0618076667 3.9920792528

H22 -2.3097941780 0.3801269135 4.7484140009

H23 2.2192079188 -1.1011075587 1.1676295949

eeZ (Conformer 2)

C1 -0.0034623404 -0.0303938396 0.0083708837

C2 0.0177823175 0.0160265608 2.5114598511

C3 2.1893286030 -0.0051368105 1.2421685715

C4 1.4723698663 0.5122928231 2.4907646723

C5 1.4594357599 0.4179230768 -0.0268698705

C6 -0.7215415369 0.4799965956 1.2551309808

H7 3.2174979418 0.3586702989 1.2256643740

H8 1.9924397737 0.1832525017 3.3899428470

H9 1.9441821242 -0.0004188474 -0.9110470504

H10 -1.7546396360 0.1256426826 1.2627498510

H11 0.0111532657 -1.0747509099 2.5442250931

H12 1.4781753528 1.6052188293 2.4899713664

H13 -0.7509947364 1.5691334438 1.2279924651

H14 -0.0490114871 -1.1197976625 -0.0092084418

H15 1.4897154522 1.5042328142 -0.1323942773

C16 -0.7262301758 0.4780430998 -1.2193209539

C17 -0.7267186803 0.4495216751 3.7412160426

O18 -1.2085683357 -0.3130298548 4.5492682802

O19 -0.8189816658 1.7178129266 -1.3678998544

O20 -1.1930039414 -0.3643652153 -2.0229888353

O21 -0.8463270267 1.7728333848 3.8757170818

H22 -1.3498004014 1.9682104641 4.6862680806

H23 2.2394428232 -1.0967429718 1.2798639196

cis-1,3-CDCA monoanion in DMSO

aaZ

C1 -0.0598527932 -0.0058525261 0.0241826123

C2 -0.0042884600 0.1043203705 2.6168917539

C3 2.1415462047 -0.0473492351 1.2526768494

C4 1.4360704296 -0.4139248735 2.5577905487

C5 1.3648567912 -0.5800384669 0.0511965470

C6 -0.8017838838 -0.2411231063 1.3414051296

H7 2.2311680294 1.0399892953 1.1798279564

H8 1.4065582655 -1.5022356389 2.6515208942

H9 1.3197387984 -1.6713924674 0.0947506445

H10 -1.0524245554 -1.3011163417 1.4020717784

H11 -0.5173030502 -0.3908849102 3.4458907642

H12 1.9933873005 -0.0350632161 3.4121623568

H13 -1.7413462516 0.3072451804 1.3366993478

H14 -0.6146630124 -0.4972130720 -0.7752848763

H15 1.8650017476 -0.3183697059 -0.8795857904

C16 0.0139939081 1.4720789050 -0.3631240406

C17 -0.0537789701 1.5616638645 3.0197872945

O18 0.9094441319 2.2494287236 3.2716088227

O19 0.3915283775 1.7291768129 -1.5350995015

O20 -0.2865383202 2.3216732375 0.5051410881

O21 -1.3006289433 2.0015841595 3.2379280016

H22 -1.2500135299 2.9213476148 3.5459980967

H23 3.1569156236 -0.4426892583 1.2520687328

aaE (H-bonded)

C1 -0.0449502837 0.0453701679 0.0005379219

C2 -0.0318097132 0.0534818879 2.6428264263

C3 2.1237634744 -0.0410757171 1.3057205786

C4 1.3976544797 -0.5185546107 2.5594066578

C5 1.3794413107 -0.5329025288 0.0682513926

C6 -0.8158987284 -0.0902804412 1.3243919933

H7 2.1892118744 1.0531666611 1.2979587950

H8 1.3393232223 -1.6090756208 2.5405635613

H9 1.3262639753 -1.6236795564 0.0976928170

H10 -1.2460699003 -1.0915023115 1.3348860298

H11 -0.5687560661 -0.5151827657 3.4003686777

H12 1.9375825729 -0.2469974636 3.4643394997

H13 -1.6617725985 0.5971766737 1.3224854099

H14 -0.5966067288 -0.5147569821 -0.7533599053

H15 1.9049350082 -0.2644203690 -0.8456637149

C16 0.0245095877 1.4535048901 -0.5843621412

C17 0.0388936230 1.4404872352 3.2656282595

O18 0.3234110225 1.5484607659 4.4505523064

O19 0.3719548368 1.5678761686 -1.7667239298

O20 -0.2798425869 2.4517514184 0.1491064861

O21 -0.2027211636 2.4981574794 2.5462634231

H22 -0.2873311591 2.3567984916 1.4780521833

H23 3.1486776010 -0.4061763577 1.3022247499

eeZ (Conformer 1)

C1 -0.0203238444 -0.0147736611 0.0127124298

C2 0.0177576560 -0.0342339367 2.5397647810

C3 2.1777949291 0.0000724412 1.2409189375

C4 1.4654110814 0.4553516137 2.5136918717

C5 1.4316014070 0.4768836083 -0.0006753782

C6 -0.7389955438 0.4310305847 1.2826086033

H7 3.2024214596 0.3745750562 1.2351533084

H8 1.9938891425 0.1022070466 3.3992025550

H9 1.9282614940 0.1314772554 -0.9089240117

H10 -1.7590386530 0.0453898783 1.2932090758

H11 -0.0171197042 -1.1262607457 2.5808226304

H12 1.4645820679 1.5470020370 2.5585633065

H13 -0.8019432826 1.5207370809 1.2828907698

H14 -0.0247878655 -1.1050454641 -0.0422281224

H15 1.4270604698 1.5696074756 -0.0322306016

C16 -0.7437118216 0.5126879247 -1.2201937037

C17 -0.7281842186 0.4877779839 3.7356911633

O18 -0.4203364338 1.4686891117 4.3734582148

O19 -1.0256708168 1.7335545017 -1.2408703933

O20 -0.9905141694 -0.3033943246 -2.1432600242

O21 -1.8314533657 -0.2163984105 4.0143738998

H22 -2.3003159605 0.2051871349 4.7550047353

H23 2.2403808511 -1.0916851197 1.2254184425

eeZ (Conformer 2)

C1 -0.0015693015 -0.0322879457 -0.0008210930

C2 0.0117814602 0.0006097136 2.5176270987

C3 2.1879691709 -0.0036448416 1.2480646233

C4 1.4696437069 0.4875149292 2.5053462430

C5 1.4558881088 0.4363642851 -0.0162075167

C6 -0.7237250050 0.4578819634 1.2534206407

H7 3.2142303876 0.3666657502 1.2409739516

H8 1.9859002093 0.1368340363 3.3992697593

H9 1.9563237078 0.0455404908 -0.9039946084

H10 -1.7523195965 0.0913279463 1.2607504734

H11 -0.0035629594 -1.0895493076 2.5656713459

H12 1.4803998767 1.5797557947 2.5309130834

H13 -0.7665600859 1.5466740075 1.2296395059

H14 -0.0278901943 -1.1225676976 -0.0270742046

H15 1.4701404707 1.5255575649 -0.0974394536

C16 -0.7358408224 0.4731799308 -1.2366123679

C17 -0.7236021340 0.4622176667 3.7448347088

O18 -1.2184165890 -0.2795020630 4.5648693640

O19 -0.8481419749 1.7149095791 -1.3670302208

O20 -1.1804980808 -0.3833032007 -2.0394015619

O21 -0.8067209698 1.7904496275 3.8608570244

H22 -1.3005752254 2.0066639202 4.6713413763

H23 2.2472352481 -1.0954521736 1.2672968978

cis-1,3-CDCA dianion in water

aa

C1 0.0334954695 -0.0965477034 0.0010140035

C2 0.0229323834 -0.0886448933 2.5051531146

C3 2.2235434560 0.0452146261 1.2537260157

C4 1.5548279639 -0.1095339597 2.6193019144

C5 1.4274146724 -0.7097466466 0.1945771015

C6 -0.4260838436 0.6648401474 1.2540860663

H7 2.2657633054 1.1007705651 0.9808200432

H8 1.8586963796 -1.0450164498 3.0888210394

H9 1.3183187034 -1.7496269466 0.5079569329

H10 -1.5084017545 0.7848192052 1.2419194150

H11 -0.3800367234 -1.0987173282 2.4494618688

H12 1.8654426056 0.6986018141 3.2769404966

H13 0.0001664839 1.6713420077 1.2710346247

H14 -0.6971692914 -0.8795244338 -0.1945525492

H15 1.9511850104 -0.7119261749 -0.7567870118

C16 -0.0450824520 0.8922405927 -1.1470419610

C17 -0.6336770545 0.5946757996 3.6729180038

O18 -0.1338884020 1.6632381041 4.0911493726

O19 -1.1913374263 1.1277791485 -1.6075848563

O20 1.0055092601 1.4594916259 -1.5278589311

O21 -1.6909647724 0.0954048474 4.1310757744

H22 3.2533593637 -0.3037113122 1.2996478123

ee

C1 0.0000000000 0.0000000000 0.0000000000

C2 0.0000000000 0.0000000000 2.5069354006

C3 2.1759627129 0.0000000000 1.2657788271

C4 1.4488808714 0.4769968181 2.5143621091

C5 1.4466962558 0.4835848959 0.0159136529

C6 -0.7360362698 0.4646872998 1.2541891207

H7 3.2079189949 0.3534720996 1.2697141013

H8 1.9409629302 0.1261316760 3.4222755092

H9 1.9553409687 0.1479468795 -0.8876481950

H10 -1.7616450192 0.0893701158 1.2581221962

H11 -0.0351308810 -1.0891801041 2.5512745940

H12 1.4507146556 1.5676920707 2.5505941523

H13 -0.7920873007 1.5548193798 1.2550911912

H14 -0.0292296346 -1.0907882338 -0.0281826930

H15 1.4435516464 1.5750773739 -0.0055149237

C16 -0.7868040750 0.5111644961 -1.1891012700

C17 -0.7449935122 0.5337574365 3.6965569230

O18 -0.6934446617 1.7655468737 3.9141351429

O19 -0.5751216926 1.6847358325 -1.5768243529

O20 -1.6489121383 -0.2585352116 -1.6833276570

O21 -1.4107496543 -0.2687626363 4.3953449129

H22 2.2101129521 -1.0926810588 1.2669476344

cis-1,3-CDCA dianion in DMSO

aa

C1 0.0340620330 -0.0713346771 -0.0133593600

C2 0.0390242503 -0.0567679164 2.5016671124

C3 2.2299540351 0.0473025522 1.2138813836

C4 1.5709399479 -0.0183800449 2.5965729038

C5 1.4050570144 -0.7270496084 0.1912175888

C6 -0.4277790075 0.6835398949 1.2484159282

H7 2.3000511039 1.0840833511 0.8822089290

H8 1.9148487802 -0.9012106214 3.1370896160

H9 1.2662123942 -1.7519513842 0.5410415814

H10 -1.5105489518 0.7890054263 1.2360161978

H11 -0.3121928672 -1.0858138489 2.4244278243

H12 1.8541647827 0.8518072306 3.1843231869

H13 -0.0133680258 1.6959646143 1.2591514763

H14 -0.7111768855 -0.8346173487 -0.2336260235

H15 1.9216587224 -0.7787695621 -0.7632754650

C16 -0.0015424011 0.9290113789 -1.1616431622

C17 -0.6586178110 0.5571068329 3.7081736967

O18 -0.1596690153 1.5875937311 4.2185112653

O19 -1.1439471688 1.2573720955 -1.5732582796

O20 1.0793289339 1.3976995650 -1.5881865902

O21 -1.7301438219 0.0159021160 4.0846563751

H22 3.2503459060 -0.3294016162 1.2641643117

ee

C1 0.0506587679 -0.0352990289 -0.0027589033

C2 0.0486683447 -0.0377039970 2.5214933768

C3 2.2301985823 -0.0120158953 1.2600062807

C4 1.4964200804 0.4507497159 2.5150893193

C5 1.4978274587 0.4551542347 0.0057062460

C6 -0.6808983786 0.4190884277 1.2590526345

H7 3.2575066045 0.3578495149 1.2615373811

H8 2.0068870858 0.1007691093 3.4136250240

H9 2.0092469922 0.1086019898 -0.8936549963

H10 -1.7050053070 0.0387902778 1.2577875239

H11 0.0309817050 -1.1283322829 2.5599077650

H12 1.4884020900 1.5416492254 2.5567502523

H13 -0.7408753996 1.5085348381 1.2599557085

H14 0.0353200854 -1.1258953192 -0.0409955964

H15 1.4888227329 1.5462477207 -0.0318005209

C16 -0.7181000143 0.4776613868 -1.2101066086

C17 -0.7201759177 0.4775217733 3.7279496744

O18 -0.6695231871 1.7082618135 3.9624994155

O19 -0.6643731459 1.7074262562 -1.4494346351

O20 -1.3875056277 -0.3561665486 -1.8717086817

O21 -1.3863040499 -0.3552757032 4.3942495122

H22 2.2872887412 -1.1040182116 1.2580046587